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A New Computational Method for non-LTE, the Linear Response Matrix

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My coauthors have done extensive theoretical and computational calculations that lay the ground work for a linear response matrix method to calculate non-LTE (local thermodynamic equilibrium) opacities. I will give briefly review some of their work and list references. Then I will describe what has been done to utilize this theory to create a computational package to rapidly calculate mild non-LTE emission and absorption opacities suitable for use in hydrodynamic calculations. The opacities are obtained by performing table look-ups on data that has been generated with a non-LTE package. This scheme is currently under development. We can see that it offers a significant computational speed advantage. It is suitable for mild non-LTE, quasi-steady conditions. And it offers a new insertion path for high-quality non-LTE data. Currently, the linear response matrix data file is created using XSN[1]. These data files could be generated by more detailed and rigorous calculations without changing any part of the implementation in the hydro code. The scheme is running in Lasnex and is being tested and developed.

The radiative properties of dense plasmas, such as stellar interiors, are usually studied using LTE methods. But we are often interested in applications that require non-equilibrium kinetic models such as low density plasmas and intermediate plasmas (e.g. laser produced plasmas) that combine high densities, a significant radiation environment and non-LTE populations.

Richard More[2] and his colleagues have done extensive work to model such non-LTE plasmas using the methods of non-equilibrium thermodynamics. They have derived a linear response matrix, $R_{\nu\nu'}$, that is *symmetric* as required by the non-equilibrium thermodynamic principles of energy conservation and minimum entropy production and by the Onsager relations and *linear* over a surprisingly large range (even up to + or - 50% changes in the photon temperature). $R_{\nu\nu'}$ is defined as follows:

$$(\kappa_\nu^e - \kappa_\nu^a)B_\nu = \frac{1}{4\pi}\int R_{\nu\nu'}\langle\frac{I_{\nu'} - B_{\nu'}}{\frac{\partial B_{\nu'}}{\partial T}}\rangle d\nu'$$

1. W.A. Lokke and W. Grasberger, UCRL-52276 (1977); G. B. Zimmerman and R. M. More, J. Quant. Spectrosc. Radiat. Transf. **23**, 517 (1979)
2. Richard More and Takako Kato, PRL **81**, 814 (1998)

To understand $R_{\nu\nu'}$ we will describe how it is calculated. Consider an ion interacting with radiation which is approximately a black body at the temperature of the free electrons. The difference between the actual radiation and the black body field causes non-equilibrium populations of excited states in the ion and leads to a net difference of emission and absorption rates. The difference of emission and absorption at frequency ν is a function of the deviation from the black body spectrum at frequency ν' and can be described as a response matrix, $R_{\nu\nu'}$. In order to generate an n x n response matrix, n non-LTE calculations are preformed. Each calculation is done with a photon spectrum that is perturbed by altering a black body equilibrium spectrum, $B_\nu(T)$ where

$$B_\nu(T) = A\frac{\nu^3}{\exp\left(\frac{\nu}{T}\right) - 1}$$

$B_\nu(T)$ is the specific intensity of radiation at frequency, ν, for a temperature, T, both in units of energy. A is a constant. The black body spectrum is altered by increasing the radiation intensity by a small factor, say 0.01, over a narrow frequency range, ν'. The net radiated power at all frequencies is then calculated. It can be positive (emission) or negative (absorption) and is found to be linearly proportional to the change in the radiation intensity, $dI_{\nu'} = I_{\nu'}-B_{\nu'}$, for small perturbations.

More and Kato[3] have studied $R_{\nu\nu'}$ for aluminum using calculations performed with the collisional-radiative (CR) model of Fujimoto and Kato[4] at near -LTE conditions and with the Livermore XSN package which is a non-LTE, screened-hydrogenic average atom model. These two "codes" give quantitative agreement good to ~20% for the linear response matrix. The symmetry of $R_{\nu\nu'}$ provides a consistency test for non-LTE models. In fact, a bug in the XSN code was found when these calculations were done and a non-symmetric matrix was obtained. Upon fixing the bug, the matrix obtained was symmetric.

How do we propose to use this formalism to produce fast non-LTE emission and absorption opacities for a radiation hydrodynamics code? It is the linearity of the response matrix that is the basis for the scheme. To implement it we must both create a data base with a non-LTE atomic physics code and then use this data base in the hydro code. Rather than creating the linear response matrix $R_{\nu\nu'}$ described, we form two similar n x n matrices. One is for emission opacities and one for absorption opacities because Lasnex requires both. Emission and absorption opacities are then calculated with a table look-up procedure.

In my work, on a pre-set material density, ρ, and temperature grid, 50 XSN calculations are performed to generate 50 x 50 matrices at each (ρ,T) point that describe the linear response of both the emission and absorption opacities at the 50 specified frequencies. The

3. ibid.

4. T. Fujimoto and T. Kato, Phys. Rev. **A 30**, 379 (1984)

LTE opacities (where $I_\nu = B_\nu$) and the opacities assuming I_ν=0 (for future work to provide realistic limiting values) are also stored in the table at each (ρ,T) point. The required data file for this case contains about one million numbers (8 megabytes using double's). The XSN calculations are done on a finer frequency mesh (300 groups). Six neighboring groups are perturbed and the results are averaged to the 50 group structure to be used in the simulation code. XSN has many parameters to set. We choose them carefully to correspond exactly to the ones that we'll use in Lasnex for comparison.

In order to avoid dividing by the exponentially small numbers in the tail of the black body distribution, we divide the perturbed distribution by dB_ν/dT, as in the definition of $R_{\nu\nu'}$. The actual values stored in the lrm (linear response matrix) table are

$$LRM_{\nu\nu'}(\rho,T) = \frac{\kappa_\nu^{NLTE}(\nu') - \kappa_\nu^{LTE}}{\left(\dfrac{I(\nu') - B(\nu')}{\dfrac{\partial}{\partial T}B(\nu')}\right)}$$

for both absorption and emission. Also we store the LTE absorption and emission opacities,

$$\left(\kappa_\nu^{aLTE}(\rho,T)\right) and \left(\kappa_\nu^{eLTE}(\rho,T)\right)$$

All of these have peen properly averaged to the course groups.

Finally, the implementation in the simulation code requires reading and storing the data from the data file and using it to calculate the non-LTE opacities. To calculate the non-LTE emission and absorption opacities from the tabular data we do log-log interpolation in (ρ,T) space for each zone and frequency on the logarithm of the LTE emission and absorption opacities and on the linear response matrices, that is, on the two n x n (50 x 50) matrices. The affect of a non-LTE photon distribution on the opacity at a given frequency, ν, is then computed by summing the linear response over all the frequencies times the corresponding perturbation of the photon intensity.

$$\kappa_\nu = \kappa_\nu^{LTE} + \sum_{\nu'} LRM_{\nu\nu'}\left(\frac{I(\nu') - B(\nu')}{\dfrac{\partial}{\partial T}B(\nu')}\right)$$

We are just inverting the process used to create the linear response data. We have found it necessary to impose a ceiling on the size of the perturbation, the $(I_{\nu'} - B_{\nu'})$ and we are still testing and developing the limits of the algorithm.

Since non-LTE XSN already runs "in-line" in Lasnex, it's easy to test the new coding to see if it is working properly, by doing the same calculation with the lrm formalism and with a full XSN non-LTE calculation. I have done that and show results for aluminum at a low density (ρ=.23 g/cc) and 1 keV in the presence of a black body photon spectrum that has been perturbed by increasing the photon intensity to double its value for all frequencies from 0.19 to 0.33 keV. The lrm results compare very well with the XSN results. (XSN averages the neighboring points in order to broaden and lower the "lines." We have not chosen to do that in our averaging process and that is evident in these plots.) Similar calculations were performed to monitor the sensitivity of the results to the interpolations in (ρ, T) and the results look very reasonable.

We have also performed simulations to model an experiment in which an aluminum slab would be placed in a hohlraum and exposed to a hot radiation spectrum at a temperature of, say 150 keV. We compared a non-LTE XSN with a lrm calculation. The two were nearly the same. The lrm took less than half the total cpu time. Larger speed-ups should be possible, but that is not our focus right now.

We are continuing to test and refine the model in hopes that it will be a useful and efficient tool for modeling non-LTE physics, especially for the very large meshes, as required for three-dimensional problems.

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New Methods for NLTE

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We explore non-equilibrium thermodynamics of non-LTE atomic kinetics in hot dense plasmas

NLTE linear response matrix

Emission – absorption

Deviation from black-body spectrum

$$\underbrace{(\kappa_\nu^e - \kappa_\nu^a)}_{\text{Emission – absorption}} B_\nu = \frac{1}{4\pi} \int R_{\nu,\nu'} \underbrace{\left\langle \frac{I_{\nu'} - B_{\nu'}}{\frac{\partial B_{\nu'}}{\partial T}} \right\rangle}_{\text{Deviation from black-body spectrum}} d\nu'$$

- **This definition fits the framework of nonequilibrium thermodynamics, so $R_{\nu,\nu'}$ should obey Onsager relations**
- **$R_{\nu,\nu'}$ is useful for transport calculations**
- **This definition leads to a large range of linear response**

$$\text{Units}\left[R_{\nu,\nu'}\right] = \frac{\text{Watts}}{\text{gram [keV]}^3}$$

$R_{\nu,\nu'}$ is not the matrix of atomic rates

- $R_{\nu,\nu'}$ is calculated from the rates but only refers to the photon spectrum

- $R_{\nu,\nu'}$ has a simple, fixed format

  — independent of ion stage
  — independent of coupling (jj, L.S, intermediate or C.I.)

- $R_{\nu,\nu'}$ has a direct relation to the transport equation and electron-photon coupling coefficient

- Applies to quasi-steady near-LTE plasma

NLTE by linear-response method*

$$R_{\nu\nu'}(\rho,T_e) = \frac{(\text{Emission} - \text{Absorption})_\nu}{(I_{\nu'} - B_{\nu'}(T_e))} \frac{\partial B_{\nu'}}{\partial T_e}$$

Actual perturbed radiation

Black-body at T_e

- $\boxed{R_{\nu\nu'} = R_{\nu'\nu}}$ Rigorous test of code; Verifies nonequilibrium thermodynamics

- The linear range is large!

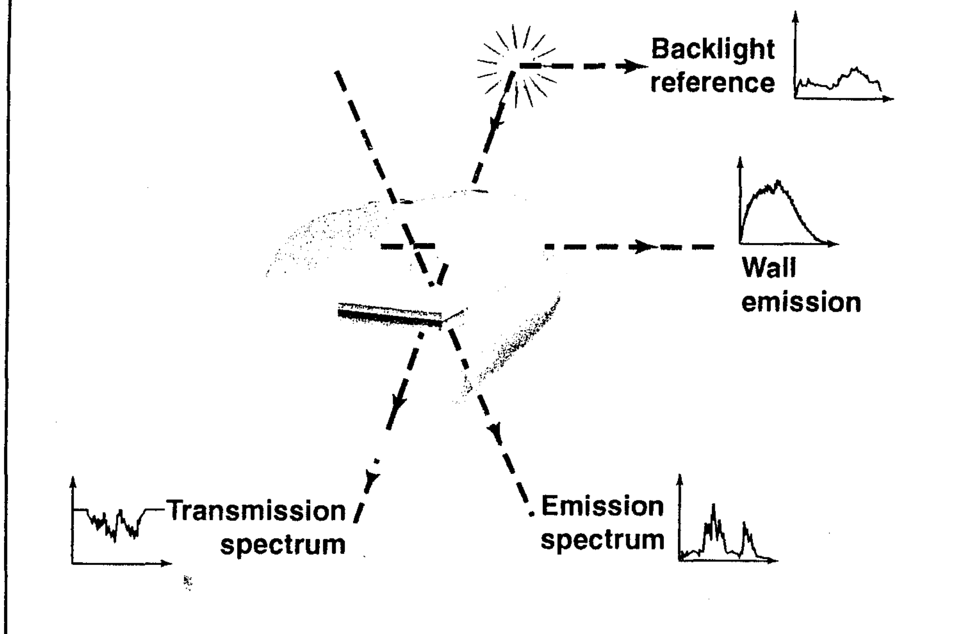
- Results from Kato-Fujimoto CR model

- Results from average-atom model

*Steady-state NLTE

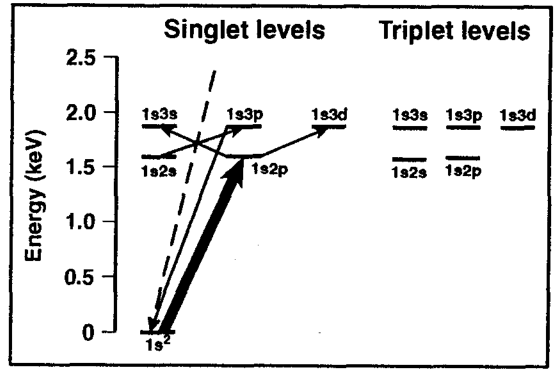
We have developed a new theory of near-LTE non-LTE plasmas

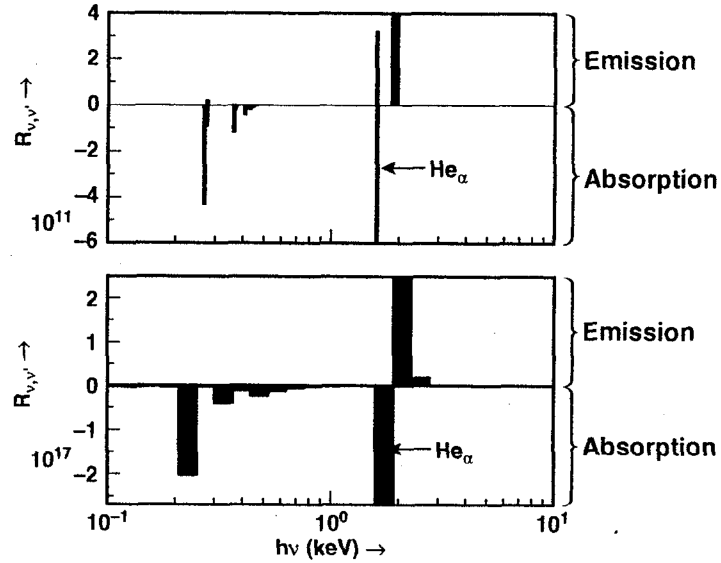
- Calculated the linear-response function for 3 NLTE codes (average atom plus NIFS and LLNL CR codes)
- Symmetric response function is a test of the NLTE code
- We find a large range of linear response
- Simple formulation of radiation transport with NLTE
- Working on a NLTE data-base system



NEAR – LTE HOHLRAUM OPACITY EXPERIMENT

Aluminum (He-like)
$N_e = 10^{20}/cm^3$ $T_e = 0.15$ keV



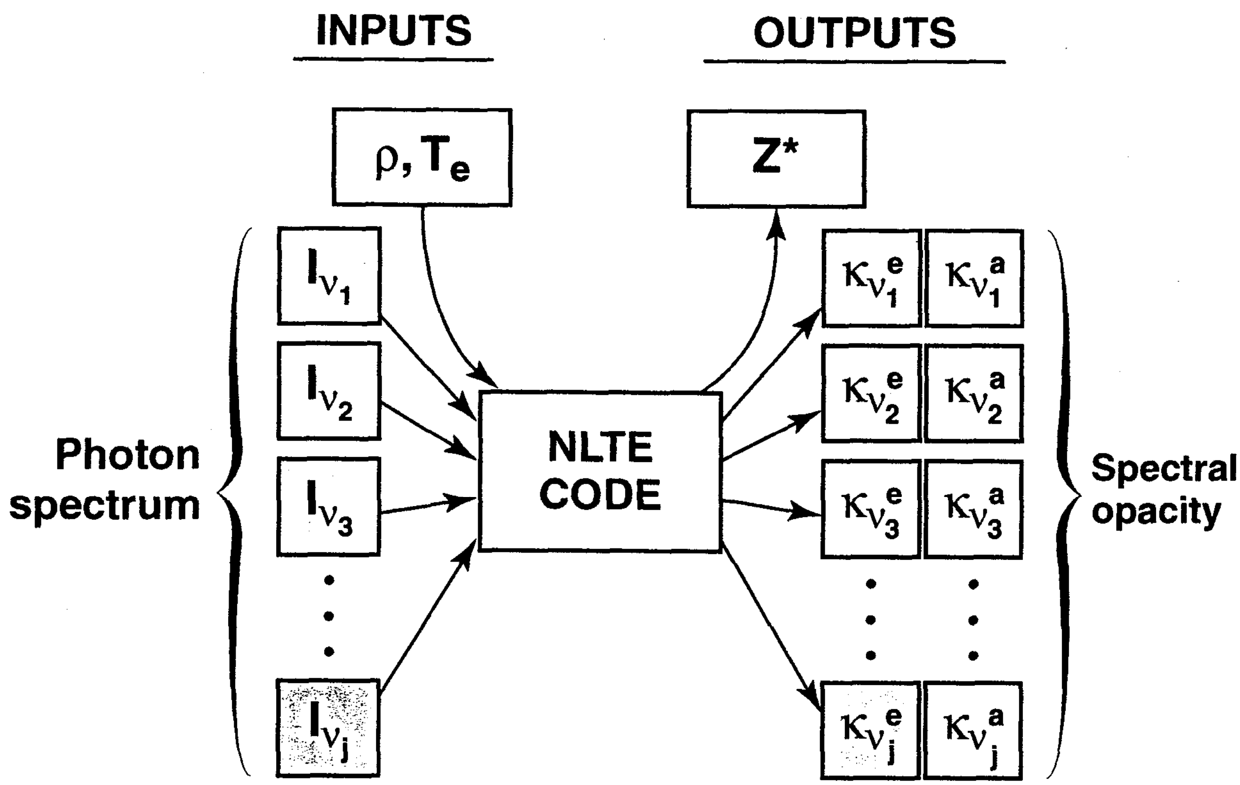


LRM Computational Chores

- "Off line" -- Build linear response matrix data file

- "On line" -- Calculate (by table look-up's) the non-LTE emission and absorption opacities, $\kappa_\nu{}^a(\rho,T)$ and $\kappa_\nu{}^e(\rho,T)$, and use them in the simulation code

Near-LTE steady-state kinetics result can be reproduced by a linear-response matrix



- The plasma simulation needs only the emission, absorption coefficients

- A vector $\{ I_\nu \}$ produces vectors $\{ \kappa_\nu{}^e \}$, $\{ \kappa_\nu{}^a \}$

  If the response were linear this would be matrix multiplication

- Near LTE, we can expect $I_\nu \approx B_\nu$ and $\kappa_\nu{}^e \approx \kappa_\nu{}^a$

  In this case,

$$\boxed{(\kappa_\nu{}^e - \kappa_\nu{}^a) \ \underline{\text{is}} \text{ a linear function of } (I_\nu - B_\nu)}$$

Screened hydrogenic model produces a symmetric response matrix $R_{\nu,\nu'}$

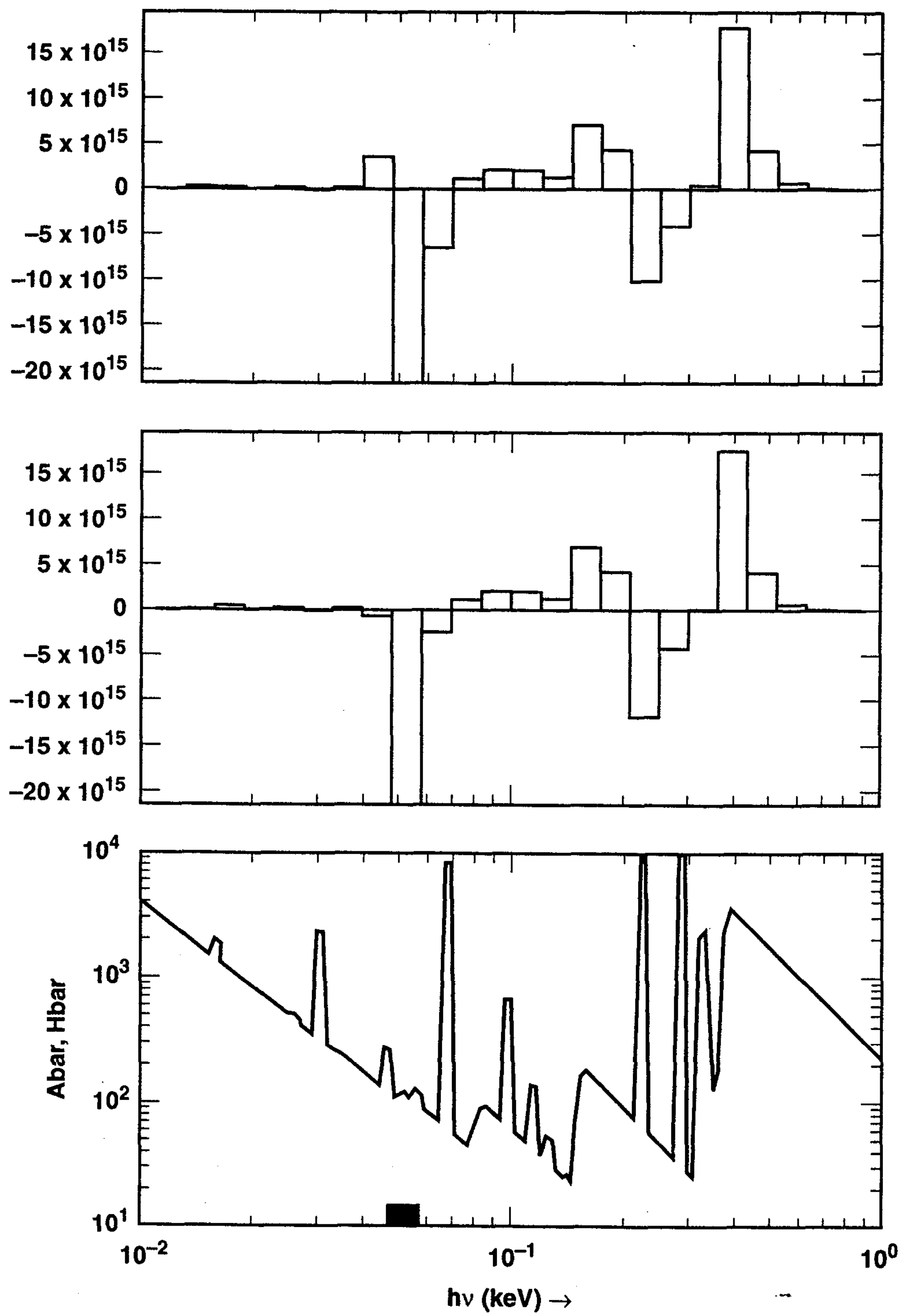
$$\begin{bmatrix} a & b & c & d \\ e & f & g & h \\ i & j & k & l \\ m & n & o & p \end{bmatrix}$$

Aluminum plasma

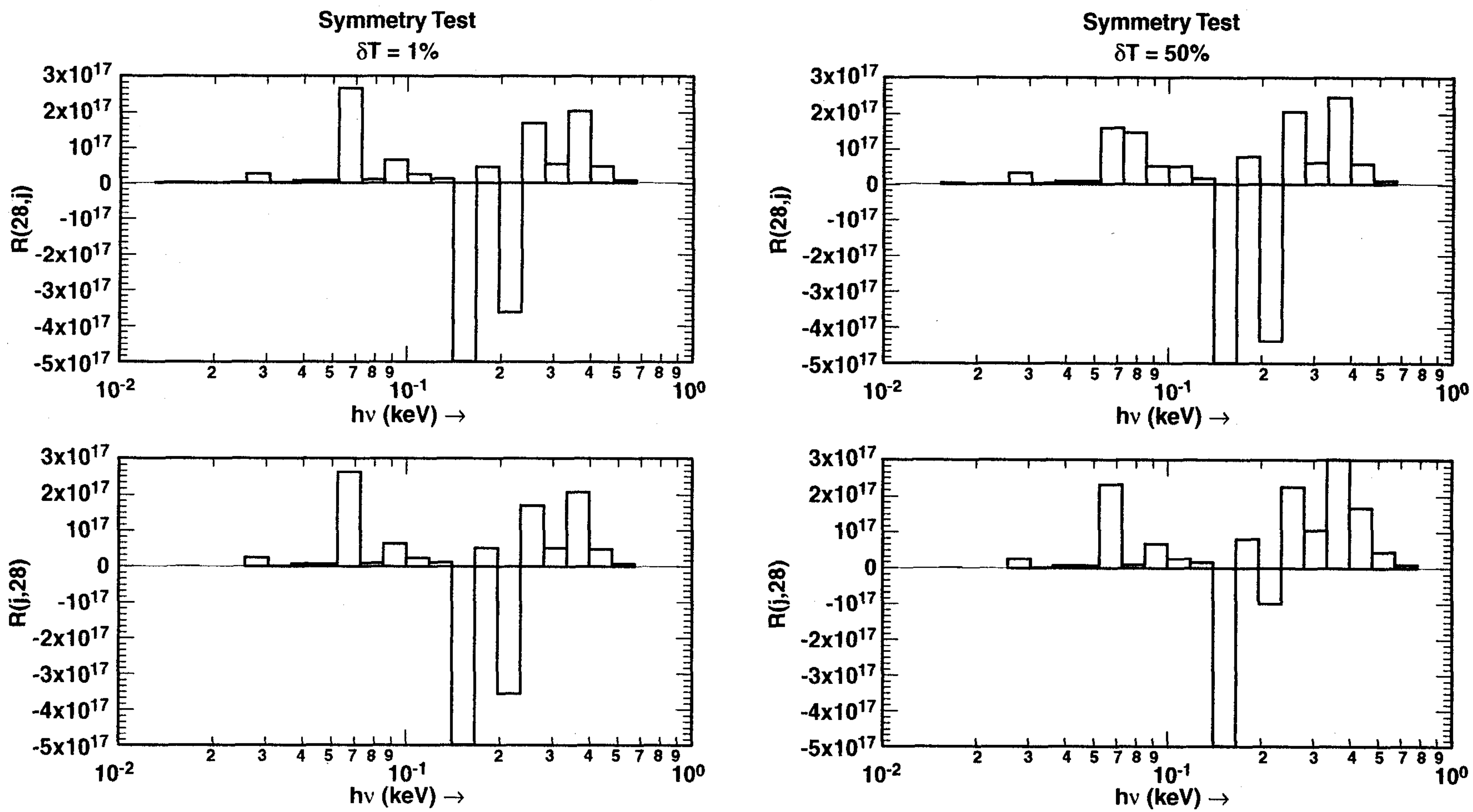
$\rho = 0.001\ g/cm^3$ $\quad T_e = 50$ eV

Change of 50 eV opacity scan of radiation perturbation

Opacity difference caused by 50 eV photon population



Response function does not depend strongly on the strength of the perturbation



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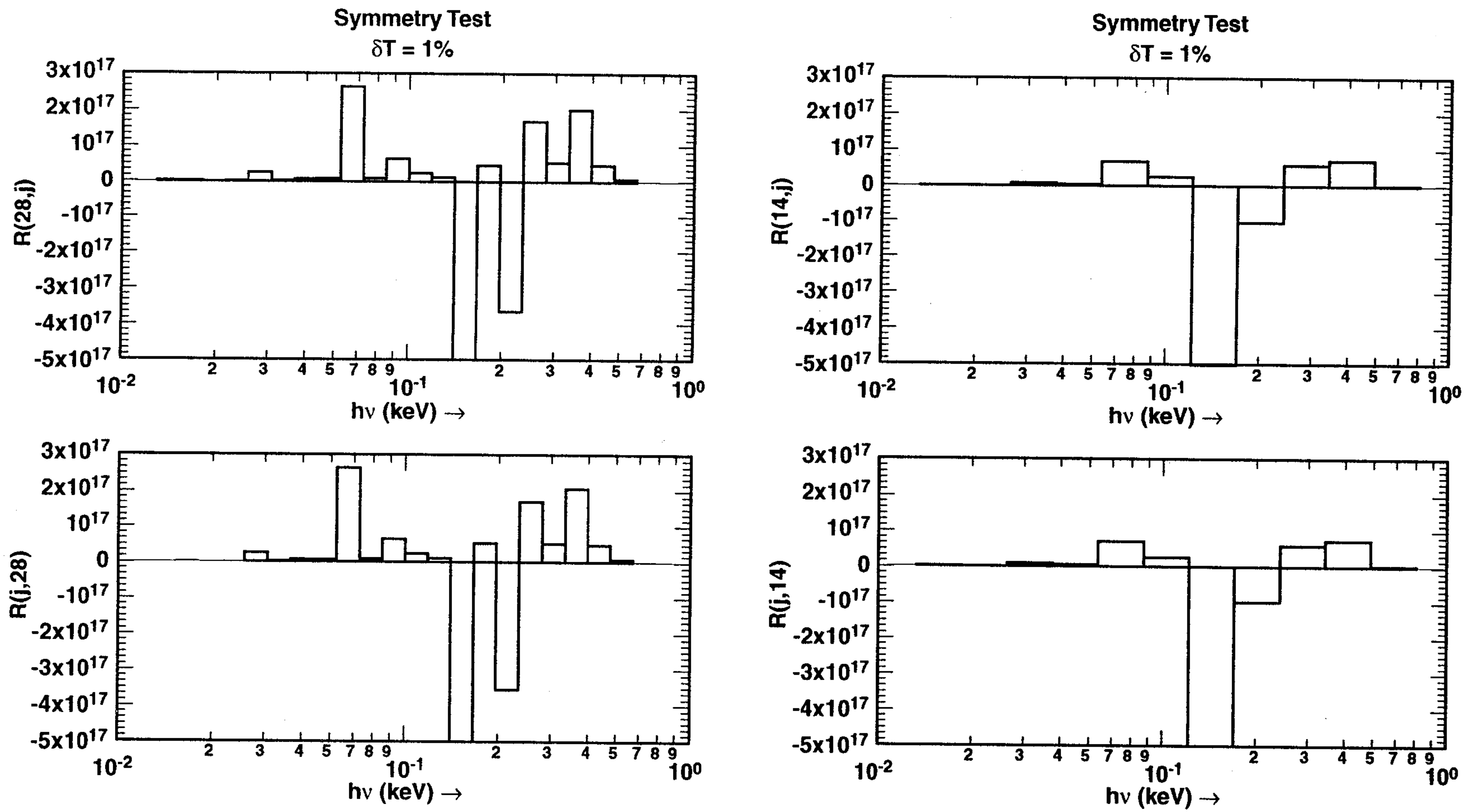
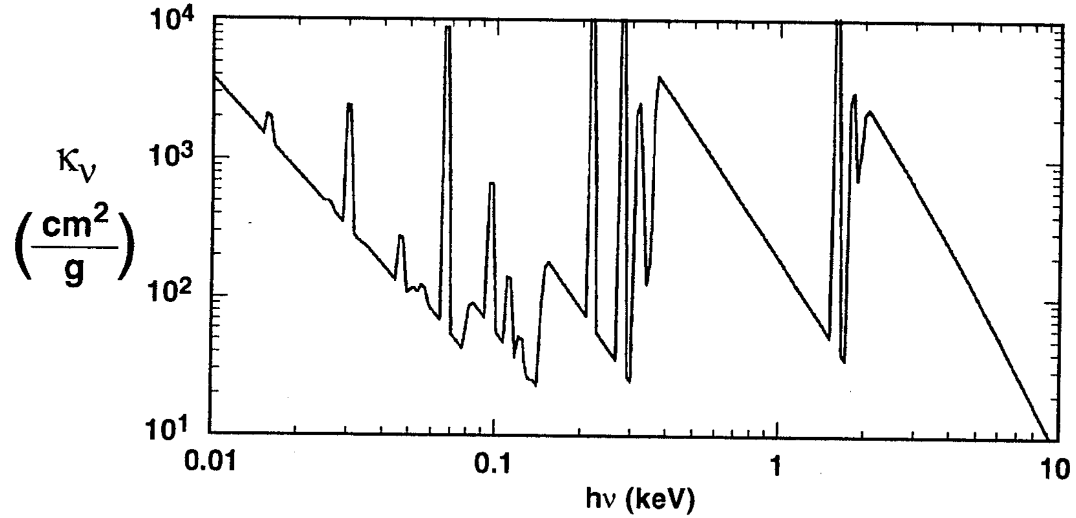
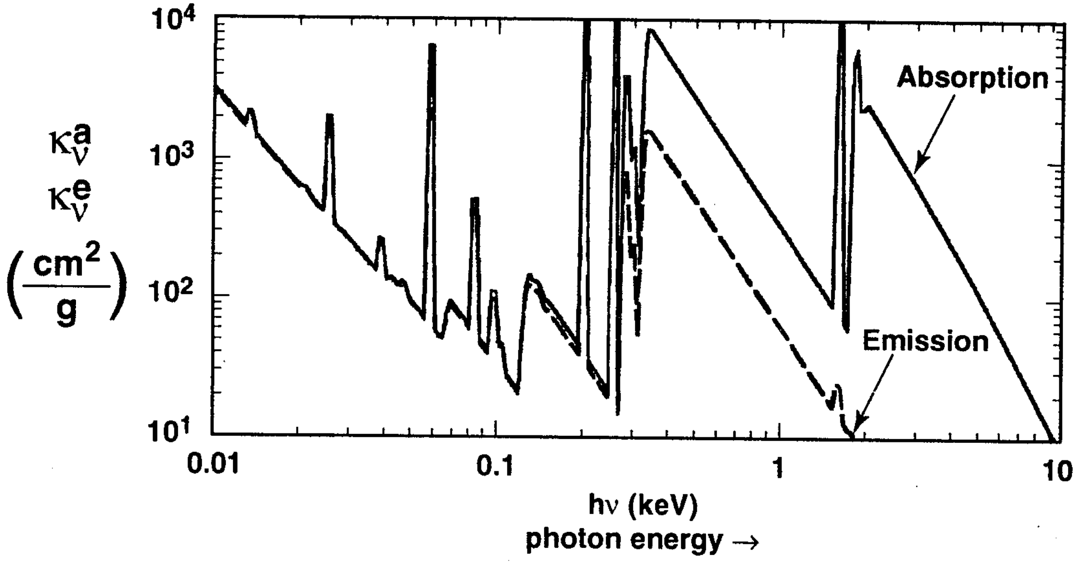
Response function does not depend strongly on the photon group sizes



NLTE conditions alter the opacity



Aluminum
LTE opacity
ρ = 0.001 g/cm^3
T_e = 50 eV
$I_\nu = B_\nu(T_e)$



NLTE
CR steady state
I_ν = 0

Building the Linear Response Matrix

- Density - Temperature Grid

  13 x 15
- Photon Frequency Grid

  50 groups

  (same for table and simulation)
- Run XSN 50 times for each (ρ,T) point (~10^4 calls) for $LRM_{\nu\nu'}$; $\kappa_\nu^{e(LTE)}$; $\kappa_\nu^{a(LTE)}$
- Table size:

  (50 x 50 x 13 x 15 x 2) + LTE opacities

  ~1 million doubles

  ~8 Megabytes

LRM Chores in the Simulation Code

- Read and store the information from the data file
  (Assume, for now, the frequency group structure in the simulation code matches the table.)

- Form the non-LTE emission and absorption opacities, $\kappa_\nu^a(\rho,T)$ and $\kappa_\nu^e(\rho,T)$. (Here is were the work is.)

- Use $\kappa_\nu^a(\rho,T)$ and $\kappa_\nu^e(\rho,T)$ for transport and coupling. That's already done in Lasnex.

Calculate LRM opacities

- Log-log interpolation in (ρ,T) space on the tablular values of $\log(\kappa_\nu^{LTE})$ and $LRM_{\nu\nu'}$

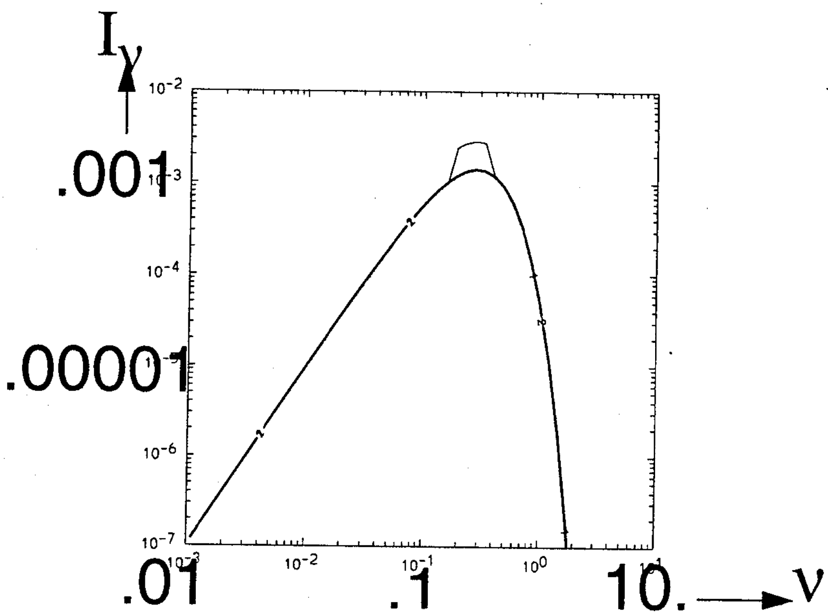
- Form the non-LTE emission and absorption opacities:

$$\kappa_\nu = \kappa_\nu^{LTE} + \sum_{\nu'} LRM_{\nu\nu'} \left(\frac{I(\nu') - B(\nu')}{\frac{\partial}{\partial T} B(\nu')} \right)$$

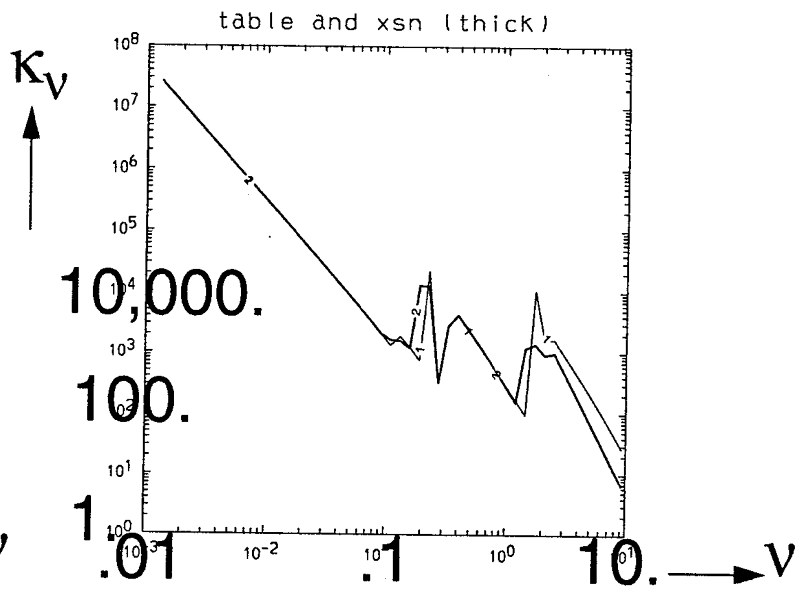
where

$I(\nu')-B(\nu') = \mathrm{sign}[\ \min\{I(\nu')-B(\nu'),\ 10*B(\nu')\}\ ,\ I(\nu')-B(\nu')\ ]$

LRM Test Calculation: Al with a non-LTE I_ν



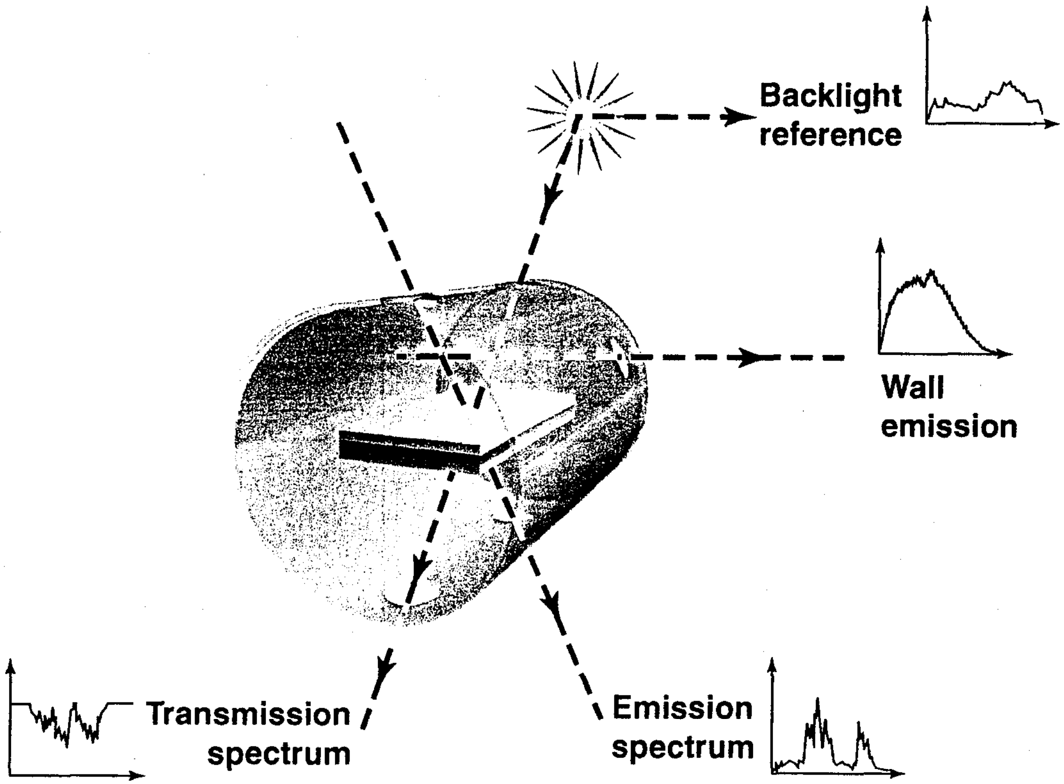
Photon distribution
[energy/cc/keV vs. keV]
Perturbed and black-body



Emission and absorption
opacities vs. frequency
LRM and XSN (2)

Al at .23 g/cc, 100 eV in a non-LTE radiation field.
[100 eV black body + 2*B_ν for ν=.19 to .33 keV]

Hohlraum opacity experiment measures emission and absorption opacities for near – LTE plasma



Quasi-steady plasma conditions

Measure:
backlight spectrum
radiation environment
absorption opacity
emission opacity

- How important are small deviations from blackbody spectrum?
- If $\kappa_\nu^e = \kappa_\nu^a$ over some spectral range, does that imply LTE?
- What are characteristic deviations from LTE?

LRM Test Calculation: Al with a non-LTE I_ν

Fractional difference $(\kappa_\nu^a-\kappa_\nu^e)/\kappa_\nu^a$ vs. frequency

LRM and XSN compare well when nlte effect is > .1% (except at that one point=> averaging)